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- Wang, L.J., P.G. Mezey and M.Z. Zgierski, Stable structures of nitrogen-rich sulfides: N<sub>3</sub>SN<sub>4</sub> and S(N<sub>4</sub>)<sub>m</sub> (m = 1–4) 369 (2003) 386
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- Zhao, J., R. Zhang and S.W. North, Oxidation mechanism of  $\delta$ -hydroxyisoprene alkoxy radicals: hydrogen abstraction versus 1,5 H-shift 369 (2003) 204
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- Zou, W., M. Lin, X. Yang and B. Zhang, Time-dependent DFT study on the electronic states of BBr 369 (2003) 214

